If the Examiner believes a telephone conference would expedite prosecution of this application, please telephone the undersigned at 650-326-2400.

Respectfully submitted,

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VERSION WITH MARKINGS TO SHOW CHANGES MADE

IN THE SPECIFICATION:

The paragraph beginning at page 10, line 30 has been amended as follows:

An asterisk indicates the transpose: $H^*(k)$, for example. A tilde over a vector indicates a 3 by 3 skew-symmetric cross product matrix: $\tilde{v}w \triangleq v \times w$. $\underline{\underline{E}}_i$ is an i by i identity matrix, and $\underline{0}_i$ is a zero vector of length i and $\underline{\underline{0}}_i$ is an i by i zero matrix.

The paragraph beginning at page 23, line 18 has been amended as follows:

The implicit Euler integration method is illustrated in the flow chart of Fig. 6 for the vector function $\dot{y} = f(y,t)$ (where $y = (q,u)$, q representing the position states and u the velocity states of the molecular system). The function f includes both the multibody system dynamics and the forces such as electrostatic attraction and repulsion, van der Waal's forces, and solvation forces. After an entry step 79, the first operation step 80 updates the Iteration matrix G. For all implicit integration methods, the Iteration matrix G has the form $G = I - \alpha J$, where I is the identity matrix, α is some scalar function of the timestep h_n, the timestep between time t_n and t_{n-1}, and J, the Jacobian given by $J \triangleq \underline{\underline{\dfrac{\partial f}{\partial y}}}$. For the implicit Euler method, $\alpha = h_n$. In passing, for additional savings in computer time, it should be noted that a very efficient method of computing Jacobian matrices from the residual form of equations is covered in previously cited co-pending U.S. Patent Appln. No. 10/053,348, entitled "METHOD FOR ANALYTICAL JACOBIAN COMPUTATION IN MOLECULAR MODELING," filed of even date and is assigned to the present assignee. As in the case of the present invention, the same referenced patent application also describes the use of internal

coordinates to describe the state of the molecular system. For example, the rotation of one part of the molecule is described with respect to another part, rather than with respect to an external referenced coordinates. This further increases computing efficiency.